Recommended Direct Simulation Monte Carlo Collision Model Parameters for Reacting Methane Flows

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While hydrocarbon combustion and gas-surface interactions have been simulated for a variety of applications in continuum solvers, such processes have been rarely investigated in Direct Simulation Monte Carlo (DSMC). Thus Variable Hard/Soft Sphere (VHS/VSS) collision parameters are not available for most molecules of interest in the decomposition of methane, a significant pyrolysis gas product and potential atmospheric species for Titan re-entries. As these properties are essential for accurate modeling of gas transport and thermochemical effects, a method must be devised to compute them for use in DSMC. In this study, the methodology outlined in Stephani et al is utilized to compute the VHS/VSS parameters by fitting the $\Omega_{(1,1)}$ and $\Omega_{(2,2)}$ collision integrals [1].

These collision integrals are typically computed from intermolecular potentials and are used in CFD simulations to calculate transport properties such as viscosity, thermal conductivity, and diffusion. This approach ensures consistency between micro-scale collisions and macro-scale transport properties. To produce the necessary collision integrals needed for the fitting routine, we utilize the method described by Laricchiuta et al, where collision integrals are computed based on the constituent particles' polarizability and effective electron number [2]. Preliminary computations of pure-species $\Omega_{(1,1)}$ and $\Omega_{(2,2)}$ collision integrals produced from the coupled approach of Stephani et al and Laricchiuta et al for methane show good agreement with those computed via available ab initio Potential Energy Surface Computations, as seen in Figure 1. Above 300K, no more than 12% deviation is observed between the two results over the temperature range of the fitted PES data [3]. Current results of this study include full *collision-specific* VSS transport properties for a complex-species mixture involving major byproducts of pure methane decomposition. Targeted final results will include a comprehensive list of VSS parameters relevant to DSMC simulations of Titan atmospheric entry, based on the reduced kinetic model of Savajano et al [4].
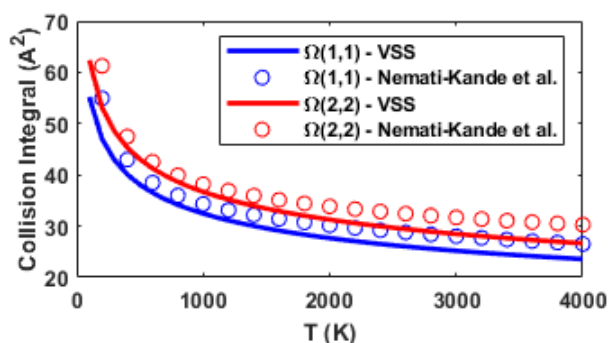

Fig. 1. Comparison of Pure-Methane Collision Integrals computed from fitted VSS Collision Parameters to those obtained from *ab initio* Potential Energy Surface calculations [4]

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